QUALITATIVE PROPERTIES OF SOME DISCRETIZED PARTIAL DIFFERENTIAL EQUATIONS AND RELIABLE FUEL CELL MODELLING

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PhD Abstract

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2011

1 Introduction

The preservation of qualitative properties of different phenomena (or of partial differential equations (PDEs)) is becoming a more and more vital requirement during the construction of reliable numerical models [6], [11], [13], [19]. For phenomena that can be mathematically described by linear PDEs of elliptic and parabolic types (such as heat conduction, reaction-diffusion, pricing of options, etc.), the most important qualitative properties are the maximum-minimum principle [14], and its special case, the non-negativity preservation.

Most differential equations can only be solved by some numerical methods, hence, it is natural that we want to use such discrete models which preserve suitable equivalents of the original properties. The PDEs are often based on real-life problems, whose solutions could be able to change or improve the life quality and style of living of the people in many areas. In the course of the recent developments of many devices, the appropriate numerical models are often playing key roles.

Nowadays, the humanity is searching for suitable solutions of the main problems of the civilization. One of the most important problems is the increasing energy hunger combined by limited resources and decreasing reserves. One promising solution to this problem could be the fuel cells, i.e., such devices that convert the chemically bounded energy (e.g., hydrogen) directly into electricity. In spite of the fact that the fuel cells are more than a hundred years old inventions, their performance and design still needs to be improved. Useful tools to develop improvements are the mathematical models, which can describe the phenomena ongoing in fuel cells. The modern mathematical description of fuel cells is based on a system of time-dependent PDEs (of parabolic type) with a (usually) nonlinear source term. By solving this problem by reliable numerical techniques, we have an efficient tool that is able to reliably model the behavior of a fuel cell, hence, without any measurements and testing instruments, we are able to perform experiments to, e.g., increasing the efficiency of the fuel cells.

2 Preliminaries and short summary of the results

The maximum principle is an important feature of scalar second order elliptic and parabolic equations, which distinguishes them from higher order equations and systems of equations [7]. The principle, in its simplest form, was first discovered for harmonic functions: any nonconstant harmonic function u (i.e., $\Delta u = 0$) assumes its minimum and maximum values only on the boundary $\partial\Omega$ of any bounded domain Ω in which $u \in C(\overline{\Omega})$,

$$\min_{\mathbf{s}\in\partial\Omega} u(\mathbf{s}) < u(\mathbf{x}) < \max_{\mathbf{s}\in\partial\Omega} u(\mathbf{s}) \quad \text{for all} \quad \mathbf{x} \in \Omega. \tag{1}$$

We have combined available theoretical estimates in order to obtain a priori two-sided bounds for the classical solutions of elliptic problems with positive reactive terms for arbitrary source functions. The validity of their discrete analogues for some well-known numerical techniques, e.g., finite difference method or finite element method has been proved.

For parabolic problems we have considered the heat conduction equation as a typical prototype for parabolic type differential equations. It is clear that the temperature in a given domain cannot be negative if the temperature was non-negative initially and was kept non-negative on the boundary of the domain as well. This property is called the non-negativity preservation. We have analyzed it for the semidiscrete solutions, and then the exact conditions has been formulated for the non-negativity preservation in one dimension for linear finite element method. Moreover, we have derived the conditions under which the bilinear finite element method is non-negativity preserving in two dimensions [2], [15], [16], [17].

We have also presented the proton exchange membrane fuel cells and its governing equations which are able to mathematically describe the operation of these devices. Two different approaches has been derived, and the preservation of some qualitative properties has been formulated as well. We have validated our theoretical results by some numerical experiments. Finally two different applications of the proton exchange membrane fuel cells have been presented [9], [10].

In the following sections we are going to present the most important results of our work.

3 Main results

3.1 Maximum principles for elliptic problems

Let Ω be a bounded domain, with Lipschitz continuous boundary $\partial\Omega$, then we are looking for a function $u \in C^2(\overline{\Omega})$ such that

$$-\Delta u + cu = f \quad \text{in} \quad \Omega, \quad \text{and} \quad u = 0 \quad \text{on} \quad \partial\Omega, \tag{2}$$

where $c(\mathbf{x})$ is the reactive coefficient (non-negative) for all $\mathbf{x} \in \overline{\Omega}$, morover $c(\mathbf{x}), f(\mathbf{x}) \in C(\overline{\Omega})$.

The classical solution of the above problem is known to satisfy the so-called maximum principle, which can be rewritten as follows

$$f(\mathbf{x}) \geq 0 \quad \text{for all} \quad \mathbf{x} \in \overline{\Omega} \implies \min_{\mathbf{x} \in \overline{\Omega}} u(\mathbf{x}) \geq 0. \tag{3}$$

In the sequel, problem (2) is considered. The key result of our work for this problem is as follows.

Theorem 3.1 [4] Let $c(\mathbf{x})$ and $f(\mathbf{x})$ in (2) be from $C(\overline{\Omega})$, moreover, additionally let

$$c(\mathbf{x}) \geq c_0 > 0 \quad \text{for all} \quad \mathbf{x} \in \overline{\Omega}, \tag{4}$$

then the following (a priori) two-sided estimates are valid for the classical solution of problem (2):

$$\min\left\{0, \min_{\xi \in \overline{\Omega}} \frac{f(\xi)}{c(\xi)}\right\} \leq u(\mathbf{x}) \leq \max\left\{0, \max_{\xi \in \overline{\Omega}} \frac{f(\xi)}{c(\xi)}\right\}, \quad \text{for any } \mathbf{x} \in \overline{\Omega}. \tag{5}$$

Remark 3.1 *Nonhomogeneous Dirichlet boundary conditions can be treated similarly* [12], *i.e., the* *following estimates hold:*

$$\min\left\{\min_{\xi\in\partial\Omega} u(\xi), \min_{\xi\in\overline{\Omega}} \frac{f(\xi)}{c(\xi)}\right\} \leq u(\mathbf{x}) \leq \max\left\{\max_{\xi\in\partial\Omega} u(\xi), \max_{\xi\in\overline{\Omega}} \frac{f(\xi)}{c(\xi)}\right\}, \quad x \in \overline{\Omega}. \tag{6}$$

It is worth emphasizing – with respect – that the very first published paper which was purely devoted to discrete maximum principles [18] *is considering the case of arbitrary Dirichlet boundary conditions, but it does not analyze another important case with nonzero source functions.*

Remark 3.2 *From the estimation* (5) *it is easy to derive the following important implication:*

$$f(\mathbf{x}) \geq 0 \ , \mathbf{x} \in \Omega \Rightarrow 0 \leq u(\mathbf{x}) \leq \max_{\xi\in\overline{\Omega}} \frac{f(\xi)}{c(\xi)}, \tag{7}$$

which is a sharper (two-sided) estimation for the unknown function u than the standard maximum principle (3) *guaranteeing only the sign of u. In what follows, we refer to* (5) *as the modified maximum principle as it makes both sharpening and also generalizing of the standard maximum principle* (3).

Remark 3.3 *Discrete maximum principles have been widely used for proving stability and finding the rate of convergence for finite difference methods and proving the convergence of finite element approximations in the maximum norm*

After discretization of (2) by, e.g., such popular numerical techniques as some finite element or finite difference method we arrive at the problem of solving an $n \times n$ system of linear algebraic equations

$$\mathbf{A}\mathbf{u} = \mathbf{F}, \tag{8}$$

where the vector of unknowns $\mathbf{u} = [u_1, \ldots, u_n]^T$ approximates the unknown solution u at certain selected points $\mathbf{x}_1, \ldots, \mathbf{x}_n$ of the solution domain Ω, and the vector $\mathbf{F} = [F_1, \ldots, F_n]^T$ approximates the values $f(\mathbf{x}_i)$, $i = 1, \ldots, n$ and $\mathbf{A} \in \mathbb{R}^{n\times n}$.
In the sequel, the entries of matrix $\mathbf{A}$ will be denoted by a_{ij}, and all matrix and vector inequalities appearing in the text are always understood component-wise.

Theorem 3.2 [3] *Let the matrix $\mathbf{A}$ in system* (8) *be strictly diagonally dominant (SDD) and monotone. Then using the notation*

$$\alpha_i(A) := |a_{ii}| - \sum_{j=1, j\neq i}^{n} |a_{ij}| > 0 \quad \text{for all} \quad i = 1, \ldots, n, \tag{9}$$

the following two-sided estimates for the entries of the unknown function $\mathbf{u}$ are valid:

$$\min\left\{0, \min_{j=1,\ldots,n} \frac{F_j}{\alpha_j(\mathbf{A})}\right\} \leq u_i \leq \max\left\{0, \max_{j=1,\ldots,n} \frac{F_j}{\alpha_j(\mathbf{A})}\right\}, \quad i = 1, \ldots, n. \tag{10}$$

Definition *We say that the solution* $\mathbf{u}$ *of system* (8) *with SDD matrix* $\mathbf{A}$ *satisfies the modified discrete maximum principle (or MDMP, in short), corresponding to the modified maximum principle* (5)*, if estimates* (10) *are valid and if, in addition,*

$$\max_{j=1,\dots,n} \frac{F_j}{\alpha_j(\mathbf{A})} \leq \max\left\{0, \max_{\mathbf{x}\in\overline{\Omega}} \frac{f(\mathbf{x})}{c(\mathbf{x})}\right\}, \tag{11}$$

$$\min_{j=1,\dots,n} \frac{F_j}{\alpha_j(\mathbf{A})} \geq \min\left\{0, \min_{\mathbf{x}\in\overline{\Omega}} \frac{f(\mathbf{x})}{c(\mathbf{x})}\right\}. \tag{12}$$

Remark 3.4 *Conditions* (11) *and* (12) *are really important in order to produce reliable (i.e. controllable) numerical approximations as, for example, linear finite difference and finite element approximations do stay within the same (a priori known) limits as those of the exact solutions they do approximate.*

To present an other major result of our work, we consider the following boundary-value problem of elliptic type. Find a function $u \in C^2(\overline{\Omega})$ such that

$$-\Delta u + cu = f \quad \text{in} \quad \Omega \quad \text{and} \quad \delta u + \frac{\partial u}{\partial n} = g \quad \text{on} \quad \partial\Omega, \tag{13}$$

where Ω is a bounded domain with Lipschitz continuous boundary $\partial\Omega$, n is the unit outward normal to $\partial\Omega$, the reactive coefficient $c(\mathbf{x}) \geq 0$ for all $\mathbf{x} \in \overline{\Omega}$, and the coefficient $\delta(\mathbf{s}) \geq 0$ for all $\mathbf{s} \in \partial\Omega$. The boundary condition in (13) is often called the third type boundary condition but also known as Newton or Robin boundary condition.

Theorem 3.3 [5] Assume that in (13) the functions $c, f \in C(\overline{\Omega})$, and the functions $\delta, g \in C(\partial\Omega)$. In addition, let

$$c(\mathbf{x}) \geq c_0 > 0 \quad \text{for all} \quad \mathbf{x} \in \overline{\Omega} \quad \text{and} \quad \delta(\mathbf{x}) \geq \delta_0 > 0 \quad \text{for all} \quad \mathbf{x} \in \partial\Omega, \tag{14}$$

where c_0 and δ_0 are (positive) constants. Then the following (a priori) two-sided estimates for the classical solution of problem (13) are valid for any $\mathbf{x} \in \overline{\Omega}$:

$$\min\left\{0, \min_{\xi\in\overline{\Omega}} \frac{f(\xi)}{c(\xi)}, \min_{\xi\in\partial\Omega} \frac{g(\xi)}{\delta(\xi)}\right\} \leq u(\mathbf{x}) \leq \max\left\{0, \max_{\xi\in\overline{\Omega}} \frac{f(\xi)}{c(\xi)}, \max_{\xi\in\partial\Omega} \frac{g(\xi)}{\delta(\xi)}\right\}. \tag{15}$$

Definition *We say that the solution* $\mathbf{u}$ *of system* (8) *with SDD matrix* $\mathbf{A}$ *satisfies the* discrete maximum principle *corresponding to the countinuous maximum principle* (15) *if estimates* (10) *are valid and if, in addition, the estimates*

$$\max_{j=1,\dots,N} \frac{F_j}{\alpha_j(\mathbf{A})} \leq \max\left\{0, \max_{\mathbf{x}\in\overline{\Omega}} \frac{f(\mathbf{x})}{c(\mathbf{x})}, \max_{\mathbf{s}\in\partial\Omega} \frac{g(\mathbf{s})}{\delta(\mathbf{s})}\right\}, \tag{16}$$

$$\min_{j=1,\dots,N} \frac{F_j}{\alpha_j(\mathbf{A})} \geq \min\left\{0, \min_{\mathbf{x}\in\overline{\Omega}} \frac{f(\mathbf{x})}{c(\mathbf{x})}, \min_{\mathbf{s}\in\partial\Omega} \frac{g(\mathbf{s})}{\delta(\mathbf{s})}\right\}, \tag{17}$$

are valid, i.e., the numerical solution remains between the same bounds as the continuous solution, or in other words the discretization is not increasing the continuous bounds.

Remark 3.5 *In the case of earlier versions of continuous and discrete maximum principles no estimates like* (11)–(12) *were, in fact, needed as one dealt there with various implications involving the sign conditions only.*

3.2 Non-negativity preservation for parabolic problems

We consider the following model problem:

$$\frac{\partial u}{\partial t} - \Delta u = 0 \quad \text{in} \quad \Omega_T = (0,T) \times \Omega, \tag{18}$$

$$u = 0 \quad \text{on} \quad \Gamma_T = (0,T) \times \partial\Omega, \tag{19}$$

$$u\big|_{t=0} = u_0 \quad \text{on} \quad \Omega, \tag{20}$$

where u stands for the temperature of the solution domain, t denotes time, and u_0 is a given initial function defined in Ω.
The most common numerical approach for solving the system (18)–(20) is the combination of separate discretizations in space and time. For the spatial one, we can apply the finite element method or the finite difference method with a given equidistant mesh size h. As a result, one can get the following Cauchy problem for the semidiscrete solution u_h, which is a time dependent vector-valued function with entries assigned to the nodes of the given mesh:

$$\frac{du_h}{dt}(t) = \Delta_h u_h(t), \;\; t \in (0,T), \tag{21}$$

where the initial value $u_h(0)$ is given, and Δ_h denotes the corresponding discrete Laplace operator (represented by a square matrix).

Theorem 3.4 *For the one- and two-dimensional problem (defined on a rectangular mesh)* (21)*, the semidiscrete numerical solutions, obtained by the finite difference discretization, preserve the non-negativity property. However, this property is not preserved, in general, by the numerical solutions resulting from the linear finite element semidiscretization.*

Applying the so-called θ-method (or weighted method) with the given time step τ and the numerical parameter $\theta \in [0,1]$ to problem (21), the following algebraic iterative equation presents the fully discretized problem

$$X_1 y^{\ell+1} = X_2 y^{\ell}, \tag{22}$$

where X_1 and X_2 are given n-by-n matrices (n denotes the ordinal number of nodes), and the vector y^ℓ represents the approximation to the vector $u_h(\ell\tau)$, moreover $y^0 = u_h(0)$ represents the given initial condition. It is clear that the matrices X_1, X_2 represent the applied numerical method. Hence, their exact form is given for our problem in the sections that are dedicated to the non-negativity preservation property of the fully discretized problem solved by finite difference and finite element methods.

For the non-negativity preservation property we have to require the condition

$$X = X_1^{-1} X_2 \geq 0, \tag{23}$$

where X is the so-called iteration matrix.

The real, uniformly continuant symmetrical tridiagonal matrices are considered with $z, w, s, p \in \mathbb{R}$

$$X_1 = z \cdot \mathrm{tridiag}(-1, 2w, -1); \quad X_2 = s \cdot \mathrm{tridiag}(1, p, 1) \tag{24}$$

with the assumptions

$$z > 0, \quad s > 0, \quad w > 1. \tag{25}$$

Theorem 3.5 [2] Under conditions (25), for arbitrary fixed n the matrix $X \in \mathbb{R}^{n\times n}$ is non-negative if and only if conditions

$$2w + p > 0 \ \text{ and } \ \gamma_{i,i} \geq \frac{1}{2w+p}, \quad i = 1, 2, \ldots, n \tag{26}$$

and

$$a(n) := \frac{\mathrm{sh}(n\vartheta)}{\mathrm{sh}((n+1)\vartheta)} \geq \frac{1}{2w+p} \tag{27}$$

are satisfied, where

$$\gamma_{i,j} = \frac{\mathrm{sh}(i\vartheta)\mathrm{sh}((n+1-j)\vartheta)}{\mathrm{sh}(\vartheta)\mathrm{sh}((n+1)\vartheta)}, \tag{28}$$

and $\vartheta = \mathrm{arch}(w)$ with $w > 1$.

Let us extend the original problem (18)-(20) by some material parameters. The more general form of the two-dimensional heat conduction equation with mixed boundary conditions on the domain $\Omega \times (0, t_{\max})$, where $\Omega := (0, L_x) \times (0, L_y)$, is

$$\begin{aligned} c(x,y)\frac{\partial u}{\partial t} &= \nabla\left(\kappa(x,y)\nabla u\right), \quad (x,y) \in \Omega,\ t \in (0, t_{\max}), \\ u|_{\Gamma_D} &= \gamma(x,y), \ \left.\frac{\partial u}{\partial n}\right|_{\Gamma_N} = 0,\ t \in [0, t_{\max}), \\ u(0,x,y) &= u_0(x,y),\ (x,y) \in \Omega, \end{aligned} \tag{29}$$

where c and κ represent the specific heat capacity and the coefficient of the thermal conductivity, respectively. The variable t denotes time, and x, y denote space variables. Moreover, $\gamma(x,y)$ is the given temperature at the part of the boundary Γ_D, which is assumed to be a non-negative real function. $\Gamma_N = \{\partial\Omega \mid y \neq 0\}$ and $\Gamma_D = \{\partial\Omega \mid y = 0\}$, where u is the temperature of the analyzed domain. Moreover Γ_N denotes a specified part of the boundary of Ω where Neumann boundary condition is imposed, and Γ_D denotes the part of the boundary where Dirichlet boundary condition is imposed to the corresponding partial differential equation. We assume that $\Gamma_D \cup \Gamma_N = \partial\Omega$ and $\Gamma_D \cap \Gamma_N = \emptyset$.

Theorem 3.6 *Let us assume that the conditions*

$$\frac{h_x h_y c}{4\left(\frac{h_x}{h_y} + \frac{h_y}{h_x}\right)(1-\theta)\kappa} \geq \tau, \tag{30}$$

and

$$\frac{h_y^2 c}{12\theta\kappa}\left(\frac{3}{2}\left(\frac{h_x^2}{h_y^2}+1\right) + \sqrt{\frac{9}{4}\left(\frac{h_x^4}{h_y^4}+1\right) + \frac{19}{2}\left(\frac{h_x^2}{h_y^2}\right)}\right) \leq \tau, \tag{31}$$

hold. Then for the problem (29) *on a rectangular domain with an arbitrary non-negative initial condition the linear finite element method results in a non-negative solution on any time level.*

Theorem 3.7 *We assume that condition* (23) *(which guarantees the non-negativity of the solution of* (22)*) holds and X_1 is SDD and monotone, then the following estimation is valid for any time level ℓ*

$$0 \leq y^{\ell+1} \leq \max\left\{0, \max_{j=1,\ldots,n} \frac{\{X_2 y^\ell\}_j}{\alpha_j(X_1)}\right\}. \tag{32}$$

3.3 Reliable modeling of fuel cells

The importance of constructing mathematical models for fuel cells is threefold. First, it leads to a better understanding of the underlying phenomena. Second, it provides a useful tool for the optimization of fuel cell systems. Third, it will be crucial to control fuel cell based applications (vehicle, backup power, etc.) in the future.

According to Kirchoff's law, the cell potential E_{cell} can be calculated by the following equation:

$$E_{\text{cell}}(t) = E_{\text{OC}}(t) - \eta^a(t) - \frac{W_{\text{mem}}}{\kappa_{\text{mem}}} I(t) - V^*(t), \tag{33}$$

where $t \in (0, t_{\max})$ denotes the time. Here $E_{\text{OC}} \approx 1.23\text{V}$ denotes the open circuit potential, which is present between the anode and cathode without the presence of any consumer. To solve the equation above we have to determine the potential losses at the particular parts of the fuel cell (anode, membrane, cathode) at a given load level.

It can be shown ([1], [8]) that the continuous mathematical model of the porous electrode under given assumptions can be transformed into the following canonical form with homogeneous initial conditions (and given Neumann type boundary conditions):

$$\partial_\delta u(\delta,\xi) = \partial_{\xi\xi} u(\delta,\xi) - \nu^2 g(u(\delta,\xi)), \quad \xi \in (0,1), \ \delta \in (0, \delta_{\max}), \tag{34}$$

where $u(\delta,\xi) := \dfrac{\alpha F}{RT}\eta(t,\xi)$ is the new unknown, the dimensionless overpotential and

$$\nu^2 = a i_0 L^2 \frac{\alpha F}{RT}\left(\frac{1}{\kappa_{\text{eff}}} + \frac{1}{\sigma_{\text{eff}}}\right) \tag{35}$$

is the dimensionless exchange current density. Moreover, ξ and δ are the new space and time variables, respectively, which are defined as

$$\xi := \frac{x}{L}, \text{ and } \delta := \frac{t}{p}, \tag{36}$$

where

$$p = \frac{C_{\text{dl}} RT}{i_0 \alpha F}\nu^2. \tag{37}$$

Theorem 3.8 *Let us assume that the condition*

$$\frac{1}{(1-\theta)\beta} \geq \tau \tag{38}$$

holds. Then for the one-dimensional problem (34)*, with arbitrary non-negative initial condition, the finite difference method results in a non-negative solution on any time level.*

Theorem 3.9 *We assume that condition* (38) *holds, then the following estimation is valid on any time level:*

$$0 \leq u^{\ell+1} \leq \max\left\{\max u^{\ell}, H(I(t))\right\}, \tag{39}$$

where $H(I(t))$ is a function which represents the time-dependent load current density, i.e., the boundary condition.

Theorem 3.10 *Let us assume that the conditions*

$$\frac{1}{\theta\left(\dfrac{6}{h^2} - \nu^2\right)} > \tau, \tag{40}$$

and

$$\frac{1}{(1-\theta)\left(\dfrac{3}{h^2} - \nu^2\right)} \leq \tau \tag{41}$$

hold. Then for the one-dimensional problem (34)*, with arbitrary non-negative initial condition, the applied linear finite element method results in a non-negative solution on any time level.*

We have obtained an explicit equation for the overpotential by eliminating the term for the potential in the solution phase without assuming constant material and kinetic coefficients. This generalizes the result for the homogeneous model, where this has been done in case of constant coefficients κ_{eff} and σ_{eff}.

$$\begin{aligned}\partial_t u(t,x) &= \partial_x(S(t,x))\frac{1}{aC_{\text{dl}}(x)}\left(-\frac{I(t)}{K} + \sigma_{\text{eff}}\partial_x u(t,x)\right)\\ &+ \frac{S(t,x)}{aC_{\text{dl}}(x)}\partial_x(\sigma_{\text{eff}}\partial_x u(t,x)) - \frac{i_0}{C_{\text{dl}}(x)K} g\left(u(t,x)\right).\end{aligned} \tag{42}$$

Theorem 3.11 *We assume that the following conditions hold:*

$$h\frac{a(x)C_{dl}(x)}{\sigma_{\mathit{eff}(x)}\partial_x S(x)} \geq \tau, \tag{43}$$

if $\partial_x S(x) \neq 0$ *and*

$$\frac{KC_{dl}(x)u(t,x)}{\frac{I(t)}{a(x)}\partial_x S(x) + i_0(x)g(u(t,x))} \geq \tau. \tag{44}$$

for all $(t,x) \in (0, t_{\max}) \times [0, L]$*, where the denominator is considered to be non-zero, i.e.,* $-\partial_x S(x) \neq I(t)a(x)i_0(x)g(u(t,x))$*. For* $u(t,x) = 0$ *the second condition in (43) is considered in the sense of limits. Then* $u^\ell \geq 0$ *yields* $f(u^\ell) \geq 0$*, and (42) results in a non-negative solution* $u^{\ell+1}$ *with any non-negative initial condition* u^ℓ*. If* $\partial_x S(x) = 0$*, then only the second condition is needed for the non-negativity preservation of the method.*

The following references list we have emphasized with bold letter the title of those papers where the main results of the thesis were published.

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